

Nuclear Shell Model Effective Interactions from Many-Body Perturbation Theory

Zhen Li

Supervisor: Nadezda A. Smirnova
Centre Etudes Nucléaires de Bordeaux Gradignan (CENBG)
CNRS/IN2P3 - Université de Bordeaux

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Outline

- ① Nuclear Many Body Problem
- ② Nuclear Shell Model
- ③ Effective Interactions from Many-Body Perturbation Theory
- ④ Summary

Nuclear Many Body Problem

A-Body Schrödinger Equation for Nucleus A

$$\hat{H}|\Psi_\alpha\rangle = E_\alpha|\Psi_\alpha\rangle$$

$$\hat{H} = \hat{T} + \hat{V} = \sum_{i=1}^A \frac{\hat{\mathbf{p}}_i^2}{2m} + \sum_{i < j}^A \hat{V}(|\mathbf{r}_i - \mathbf{r}_j|)$$

Nucleon-Nucleon Interactions

- **Chiral Potentials:** from chiral effective field theory (χ EFT), Machleidt et al., Phys. Rep. 503, 1 (2011)
- **Bonn Potentials:** based on meson-exchange models (π , η , $\rho(770)$, $\omega(782)$), Machleidt et al., Phys. Rep. 149, 1 (1987), Machleidt, Phys. Rev. C 63, 024001 (2001)
- **Daejeon16 Potential:** based on renormalized chiral potential N³LO, fitted to energies of 11 states up to $A = 16$, Shirokov et al., Phys. Lett. B 761, 87 (2016)
- **Argonne Potentials:** Wiringa et al., Phys. Rev. C 51, 38 (1995)

Nuclear Many Body Problem

Many-Body Methods for Nuclear System

- ▶ Monte-Carlo methods (VMC, GFMC, AFDMC, etc.)
 - J. Carlson et al., Rev. Mod. Phys. 87, 1067 (2015).
- ▶ Configuration Interaction (CI) methods (SM, NCSM, CC, IM-SRG)
 - E. Caurier et al., Rev. Mod. Phys. 77, 427 (2005).
 - B. R. Barrett, et al., Prog. Part. Nucl. Phys. 69, 131 (2013).
 - G. Hagen, et al., Rep. Prog. Phys. 77, 096302 (2014).
 - H. Hergert et al., Phys. Rep. 621, 165 (2016).
- ▶ Self-Consistent Green's Function (SCGF) method
 - W. H. Dickhoff et al., Prog. Part. Nucl. Phys. 52, 377 (2004).
- ▶ Many-Body Perturbation Theory (MBPT)
 - A. Tichai et al., Front. Phys. 8, 164 (2020).
- ▶ Density Functional Theory (DFT)
 - M. Bender et al., Rev. Mod. Phys. 75, 121 (2003).
- ▶ HF, GCM, AMD, ...

Nuclear Many Body Problem: NCSM

Hamiltonian

$$H = T + V = \textcolor{blue}{T} + \textcolor{blue}{U} + \textcolor{red}{V} - \textcolor{red}{U} = H_0 + H_1$$

$$H_0|\Phi_i\rangle = \mathcal{E}_i|\Phi_i\rangle, \quad i = 1, 2, 3, \dots, d$$

- U : auxiliary potential, providing approximately mean-field potential
- H_0 : Hamiltonian can be solved exactly
- H_1 : “residual” nucleon-nucleon interaction

A-Body Harmonic Oscillator Basis

$$\hat{H}_0|\Phi_i\rangle = \mathcal{E}_i|\Phi_i\rangle, \quad \hat{H}_0 = \hat{T} + \hat{U} = \sum_{i=1}^A \left\{ \frac{\hat{\mathbf{p}}_i^2}{2m} + \frac{1}{2}m\omega^2 \mathbf{r}_i^2 \right\}$$

$$|\Phi_i\rangle = \frac{1}{\sqrt{A!}} \mathcal{A} \left\{ \prod_{\alpha=i_1}^{i_A} |\phi_\alpha\rangle \right\}_i = [c_{i_1}^\dagger c_{i_2}^\dagger \cdots c_{i_A}^\dagger]_i |c\rangle, \quad \mathcal{E}_i = \sum_{\alpha=i_1}^{i_A} \varepsilon_\alpha$$

- single-particle states $\{|\phi_{i_1}\rangle, |\phi_{i_2}\rangle, \dots, |\phi_{i_A}\rangle\}$ are occupied by A nucleons
- A -body basis $\{|\Phi_i\rangle, i = 1, 2, \dots, d = \infty\}$ spans the Hilbert space (model space) for the A -body system

Nuclear Many Body Problem: NCSM

Diagonalization

$$\hat{H}|\Psi_\alpha\rangle = E_\alpha|\Psi_\alpha\rangle, \quad |\Psi_\alpha\rangle = \sum_{j=1}^d c_j^{(\alpha)}|\Phi_j\rangle, \quad \Rightarrow \sum_{i=1}^d \langle\Phi_i|\hat{H}|\Phi_j\rangle c_j^{(\alpha)} = E_\alpha c_i^{(\alpha)}$$

$$\bar{H} = \begin{bmatrix} H_{11} & H_{12} & H_{13} & \cdots & H_{1d} \\ H_{21} & H_{22} & H_{23} & \cdots & H_{2d} \\ H_{31} & H_{32} & H_{33} & \cdots & H_{3d} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ H_{d1} & H_{d2} & H_{d3} & \cdots & H_{dd} \end{bmatrix}, \text{ where } H_{ij} \equiv \langle \Phi_i | H | \Phi_j \rangle$$

► Harmonic Oscillator Basis for ^{18}O

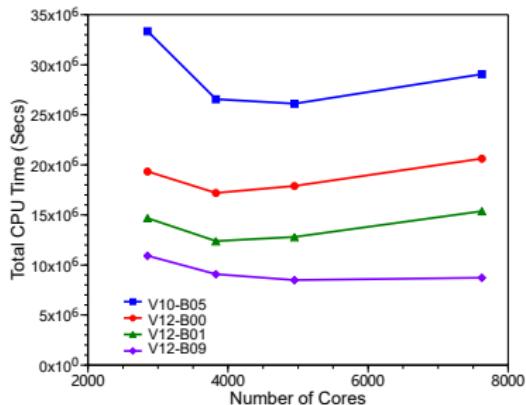
Nuclear Many Body Problem: NCSM

► N_{\max} Truncation of Basis in No Core Shell Model:

N_{\max} : maximal allowed Harmonic Oscillator excitations above the lowest configuration

Table of storage requirements for the nonzero matrix elements of the many-body Hamiltonian for a range of applications. The notation TB, PB and EB represent Terabytes (10^{12} bytes), Petabytes (10^{15} bytes) and Exabytes (10^{18} bytes), respectively. Roughly speaking, entries up to 400 TB imply Petascale computational facilities, while entries above 1PB imply Exascale computational facilities will likely be required.

Nucleus	N_{\max}	Dimension	2-body	3-body	4-body
^6Li	12	$4.9 \cdot 10^6$	0.6 GB	33 TB	590 TB
^{12}C	8	$6.0 \cdot 10^8$	4 TB	180 TB	4 PB
^{12}C	10	$7.8 \cdot 10^9$	80 TB	5 PB	140 PB
^{16}O	8	$9.9 \cdot 10^8$	5 TB	300 TB	5 PB
^{16}O	10	$2.4 \cdot 10^{10}$	230 TB	12 PB	350 PB
^8He	12	$4.3 \cdot 10^8$	7 TB	300 TB	7 PB
^{11}Li	10	$9.3 \cdot 10^8$	11 TB	390 TB	10 PB
^{14}Be	8	$2.8 \cdot 10^9$	32 TB	1100 TB	28 PB
^{20}C	8	$2 \cdot 10^{11}$	2 PB	150 PB	6 EB
^{28}O	8	$1 \cdot 10^{11}$	1 PB	56 PB	2 EB



Total CPU time of ^{13}C NCSM calculation ($N_{\max} = 6$) with chiral NN plus NNN potential, from J. P. Vary et al., J. Phys.: Conf. Ser. 180, 012083 (2009).

B. R. Barrett et al., Prog. Part. Nucl. Phys. 69, 131 (2013).

Shell Model

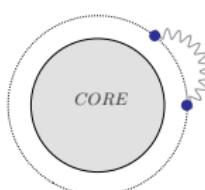
► Approximations in Shell Model (Interacting Shell Model, Shell Model with a Core, or Valence Shell Model):

- ① separate the model space into three parts: *Filled Space*, *Valence Space* and *Empty Space*
- ② only consider valence nucleons moving in the *Valence Space*

N	d_N	$\sum_N d_N$	Shells	Parity
⋮	⋮	⋮	⋮	⋮
9	110	440	$0l, 1j, 2h, 3f, 4p$	–
8	90	330	$0k, 1i, 2g, 3d, 4s$	+
7	72	240	$0j, 1h, 2f, 3p$	–
6	56	168	$0i, 1g, 2d, 3s$	+
5	42	112	$0h, 1f, 2p$	–
4	30	70	$0g, 1d, 2s$	+
3	20	40	$0f, 1p$	<i>Empty Space</i> –
2	12	20	$0d, 1s$	<i>Valence Space</i> +
1	6	8	$0p$	<i>Filled Space</i> –
0	2	2	$0s$	+

For example (^{18}O):

- *Filled Space*: $0s$ and $0p$ shells, with $4 + 12 = 16$ nucleons (being inert **core**, double magic nucleus)
- *Valence Space*: $0d-1s$ shell, with 2 nucleons (the so-called **valence nucleons**)
- *Empty Space*: other shells, without nucleons



Shell Model

► Original *A*-Body Problem:

$$\hat{H}|\Psi_\alpha\rangle = E_\alpha |\Psi_\alpha\rangle$$

► Shell Model: reduce the *A*-body problem to valence-particle problem

$$\hat{H}_{\text{eff}}^{(v)}|\Psi_\alpha^{\text{P}}\rangle = (E_\alpha - E_c)|\Psi_\alpha^{\text{P}}\rangle$$

- $\hat{H}_{\text{eff}}^{(v)}$: effective Hamiltonian of valence nucleons
- $|\Psi_\alpha^{\text{P}}\rangle$: wavefunctions of valence nucleons
- E_α : energies of nucleus *A*
- E_c : ground state energy of the core nucleus

Shell Model Effective Interactions

Effective Hamiltonian for the Shell Model

$$H_{\text{eff}} = \sum_{\alpha} \varepsilon_{\alpha} c_{\alpha}^{\dagger} c_{\alpha} + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V_{\text{eff}} | \gamma\delta \rangle c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\delta} c_{\gamma}$$

- ε_{α} : single-particle energy, usually taken from experiment
- V_{eff} : effective interaction

Effective Interaction V_{eff}

► Empirical Effective Interaction:

- p -shell: Cohen-Kurath
- sd -shell: USD, USDB¹

► Microscopic Effective Interaction (from bare nucleon-nucleon interaction):

- **Many-Body Perturbation Theory (MBPT)**: from 60s, see M. Hjorth-Jensen et al., Phys. Rep. 261, 125 (1995), L. Coraggio et al., Prog. Part. Nucl. Phys. 62, 135 (2009), and references therein
- **No-Core Shell Model**: A. F. Lisetskiy et al., Phys. Rev. C 78, 044302 (2008), E. Dikmen et al., Phys. Rev. C 91, 064301 (2015), N. A. Smirnova et al., Phys. Rev. C 100, 054329 (2019)
- **Coupled Cluster**: G. R. Jansen et al., Phys Rev Lett. 113, 142502 (2014) and Phys. Rev. C 94, 011301 (2016), Sun et al., Phys. Rev. C 98, 054320 (2018)
- **In-Medium Similarity Renormalization Group**: S. K. Bogner et al., Phys Rev Lett. 113, 142501 (2014), S. R. Stroberg, et al., Phys Rev Lett. 118, 032502 (2017).

¹USDB is the most accurate effective interaction in sd -shell

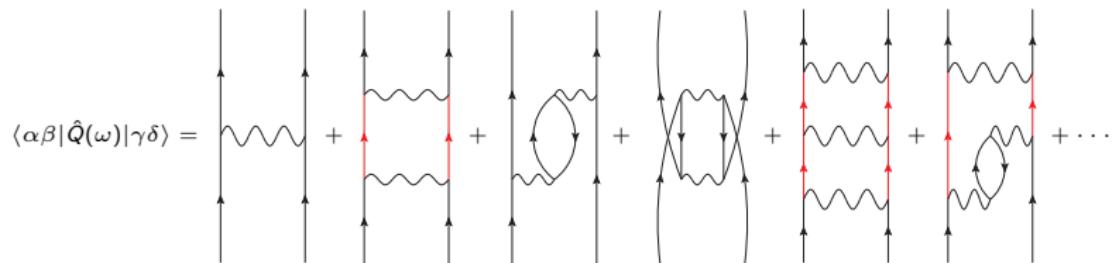
Effective Interactions from MBPT

Krenciglowa-Kuo Iteration Equation¹

$$V_{\text{eff}}^{(n)} = \hat{Q}(\omega) + \sum_{m=1}^{\infty} \hat{Q}_m(\omega) \left\{ V_{\text{eff}}^{(n-1)} \right\}^m, \quad V_{\text{eff}}^{(0)} = \hat{Q}(\omega)$$

\hat{Q} -Box from MBPT¹: valence-linked irreducible diagrams

$$\langle \alpha \beta | \hat{Q}(\omega) | \gamma \delta \rangle = \langle \text{CORE} | c_\beta c_\alpha H_1(t=0) U(0, -\infty) c_\gamma^\dagger c_\delta^\dagger | \text{CORE} \rangle_v$$



¹ see T. T. Kuo and E. Osnes, *Folded-diagram theory of the effective interaction in nuclei, atoms and molecules*. Springer-Verlag (1990), M. Hjorth-Jensen et al., *Phys. Rep.* 261, 125 (1995) and references therein.

Effective Interactions from MBPT

► Diagram Expressions:

$$\begin{array}{c} \left| \begin{array}{cc} \alpha & \beta \\ \downarrow & \downarrow \\ \text{wavy} & \\ \uparrow & \uparrow \\ \gamma & \delta \end{array} \right| = \langle \alpha\beta | V | \gamma\delta \rangle, \quad \left| \begin{array}{cc} \alpha & \beta \\ \downarrow & \downarrow \\ p_1 & p_2 \\ \text{wavy} & \\ \uparrow & \uparrow \\ \gamma & \delta \end{array} \right| = \frac{1}{2} \sum_{p_1 p_2} \frac{\langle \alpha\beta | V | p_1 p_2 \rangle \langle p_1 p_2 | V | \gamma\delta \rangle}{\varepsilon_\gamma + \varepsilon_\delta - \varepsilon_{p_1} - \varepsilon_{p_2}}, \quad \left| \begin{array}{cc} \alpha & \beta \\ \downarrow & \downarrow \\ \text{wavy} & \\ \text{loop} & \\ \uparrow & \uparrow \\ \gamma & \delta \end{array} \right| = \sum_{ph} \frac{\langle \alpha h | V | \gamma p \rangle \langle p\beta | V | h\delta \rangle}{\varepsilon_\delta + \varepsilon_h - \varepsilon_p - \varepsilon_\beta}, \dots \end{array}$$

Matrix Element of Effective Interaction V_{eff}

$$\langle \alpha\beta | V_{\text{eff}} | \gamma\delta \rangle = \langle \alpha\beta | V | \gamma\delta \rangle + \frac{1}{2} \sum_{p_1 p_2} \frac{\langle \alpha\beta | V | p_1 p_2 \rangle \langle p_1 p_2 | V | \gamma\delta \rangle}{\varepsilon_\gamma + \varepsilon_\delta - \varepsilon_{p_1} - \varepsilon_{p_2}} + \sum_{ph} \frac{\langle \alpha h | V | \gamma p \rangle \langle p\beta | V | h\delta \rangle}{\varepsilon_\delta + \varepsilon_h - \varepsilon_p - \varepsilon_\beta} + \dots$$

- $|\alpha\rangle, |\beta\rangle, |\gamma\rangle, |\delta\rangle \in \text{Valence Space}$,
- $|p_1\rangle, |p_2\rangle \in \text{Empty Space}$, $|p\rangle \in \text{Valence Space or Empty Space}$
- $|h\rangle \in \text{Filled Space}$

► Effective Interaction V_{eff} Comes from

- interaction V between valence nucleons in valence space
- interaction V between excited nucleons in empty space
- interaction V between valence nucleons and nucleons in the core
- ...

Results: *sd*-Shell Effective Interactions

DJ16-2: using MBPT (2nd order, $N_{\max} = 2$) with Daejeon16 potential¹

2^*T_z	2^*J	a^2	b	c	d	$\langle ab; J V_{\text{eff}} cd; J \rangle$
-2	0	205	205	205	205	-2.7234
-2	0	205	205	203	203	-3.6876
-2	0	205	205	1001	1001	-1.0611
-2	0	203	203	205	205	-3.6876
-2	0	203	203	203	203	-1.1277
...

DJ16-4: using MBPT (2nd order, $N_{\max} = 4$) with Daejeon16 potential

2^*T_z	2^*J	a	b	c	d	$\langle ab; J V_{\text{eff}} cd; J \rangle$
-2	0	205	205	205	205	-2.6805
-2	0	205	205	203	203	-3.5751
-2	0	205	205	1001	1001	-1.0801
-2	0	203	203	205	205	-3.5751
-2	0	203	203	203	203	-1.1246
...

- **CD-Bonn** effective interaction³: using MBPT (2nd order, $N_{\max} = 2$) with CD-Bonn potential
- **N3LO** effective interaction⁴: using MBPT (2nd order, $N_{\max} = 2$) with N3LO potential

¹see A. M. Shirokov et al., Phys. Lett. B 761, 87 (2016) for Daejeon16 potential

² $|a\rangle \equiv |n_a, l_a, j_a\rangle$ labeled by $1000n_a + 100l_a + 2j_a$

³see R. Machleidt, Phys. Rev. C 63, 024001 (2001) for CD-Bonn potential

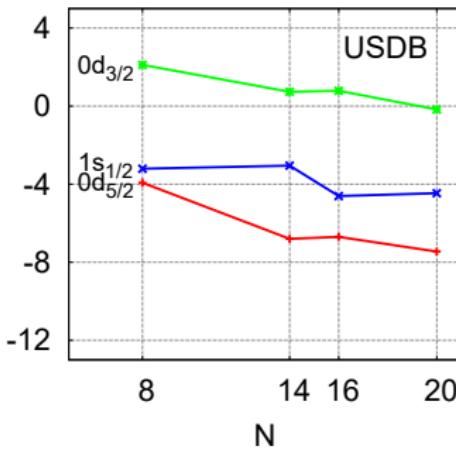
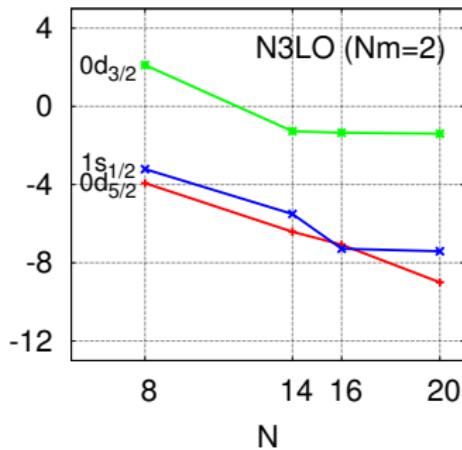
⁴see R. Machleidt and D. R. Entem, Phys. Rep. 503, 1 (2011) and references therein for N3LO potential

Results: *sd*-Shell Effective Interactions

Effective Single-Particle Energy¹: single particle energy in the mean filed approximation

$$\tilde{\varepsilon}_k^\rho = \varepsilon_k^\rho + \sum_{k' \neq k} V_{kk'}^{\rho\rho'} n_{k'}^{\rho'}, \quad V_{kk'}^{\rho\rho'} = \frac{\sum_J \langle k_\rho k'_{\rho'} | V | k_\rho k'_{\rho'} \rangle_J (2J+1)}{\sum_J (2J+1)}$$

► Neutron ESPEs for O isotopes²:



¹R. K. Bansal and J. B. French, Phys. Lett. 11, 145 (1964), T. Otsuka et al., Prog. Part. Nucl. Phys. 47, 319 (2001), N. A. Smirnova et al., Phys. Lett. B 686, 109 (2010)

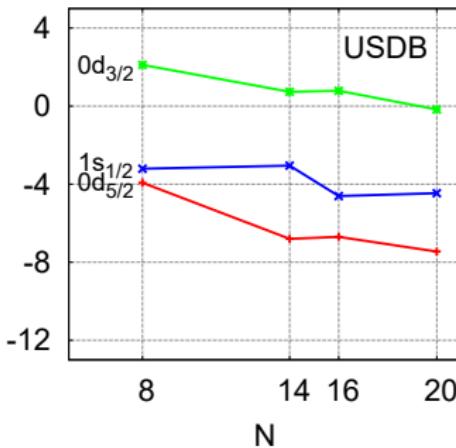
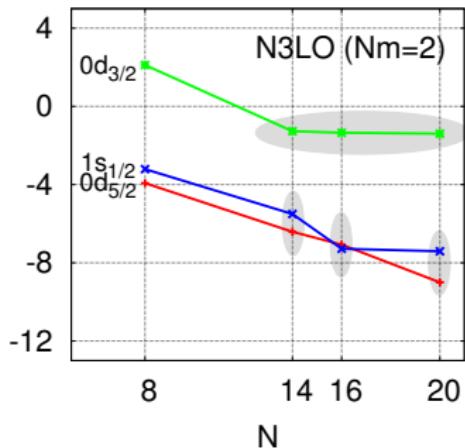
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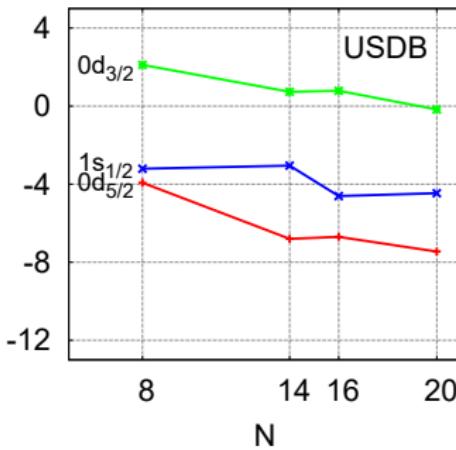
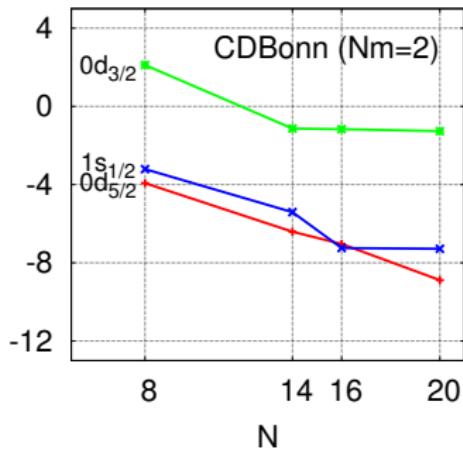
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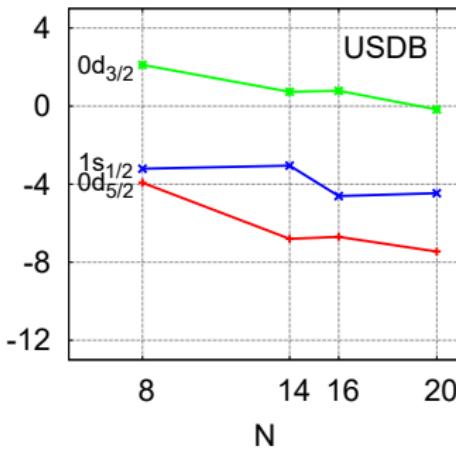
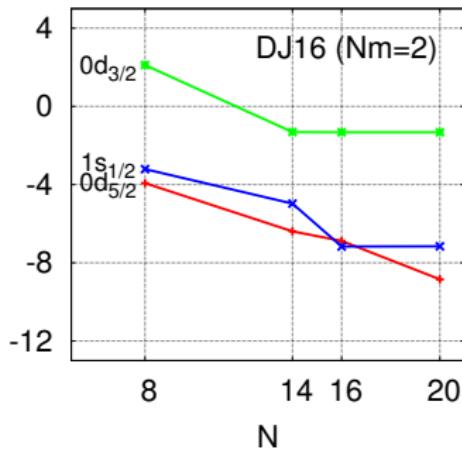
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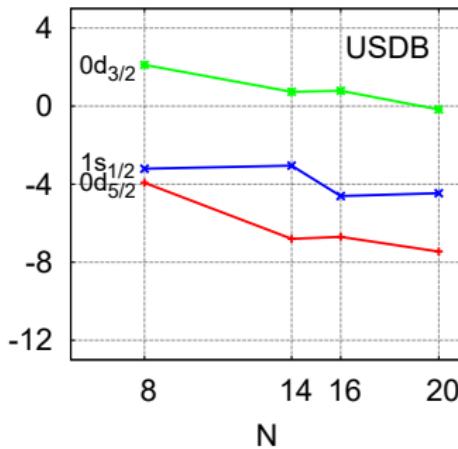
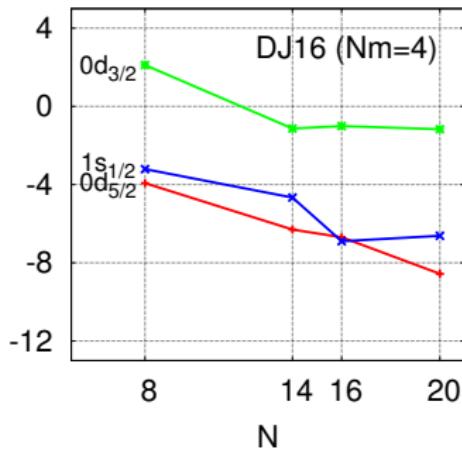
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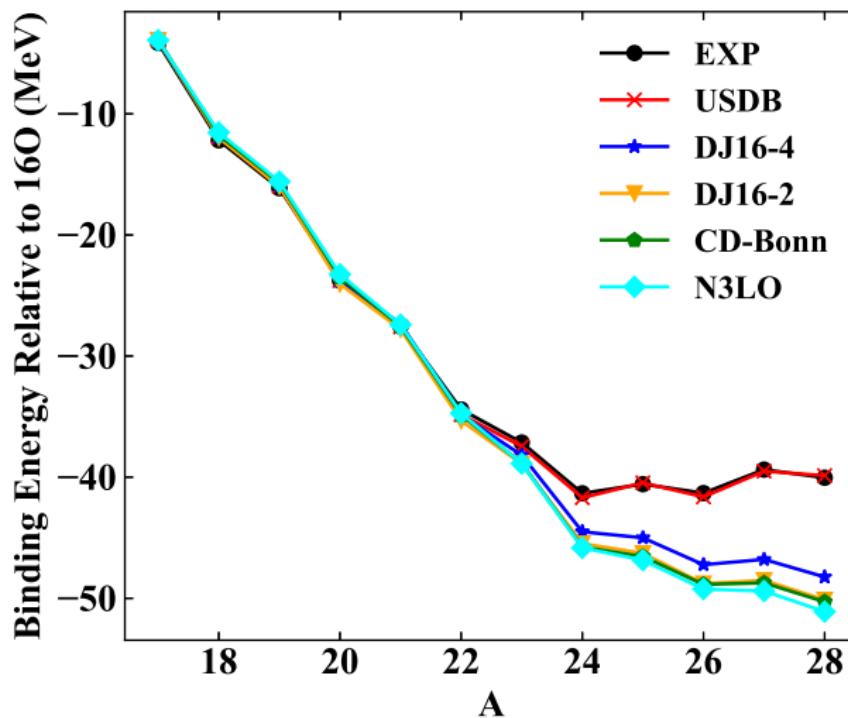


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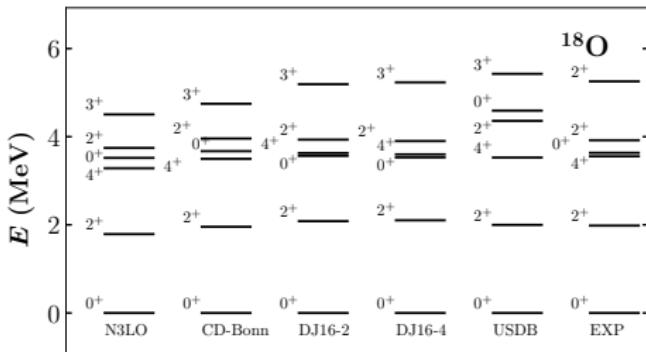
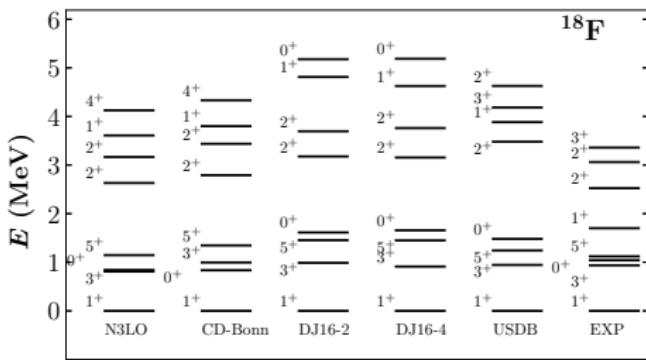
Results: *sd*-Shell Effective Interactions

- Binding Energies of O isotopes relative to ^{16}O :



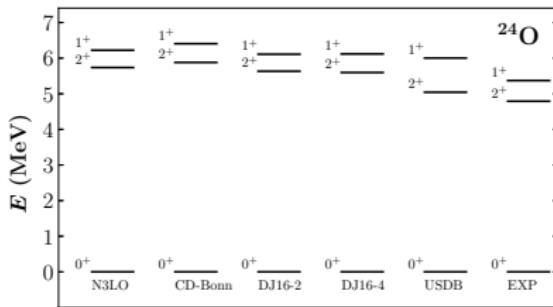
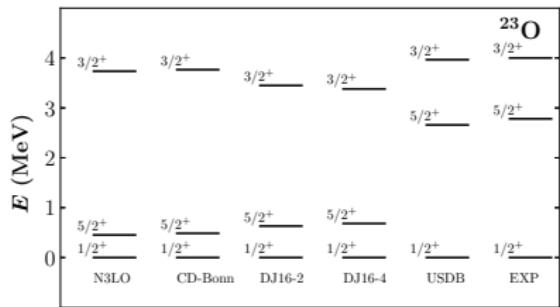
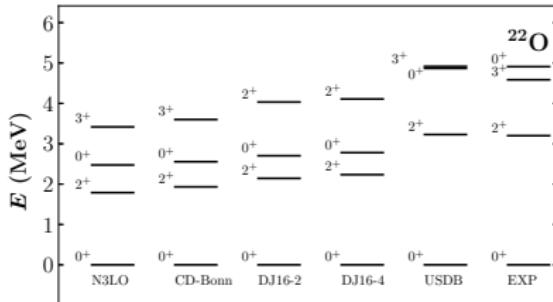
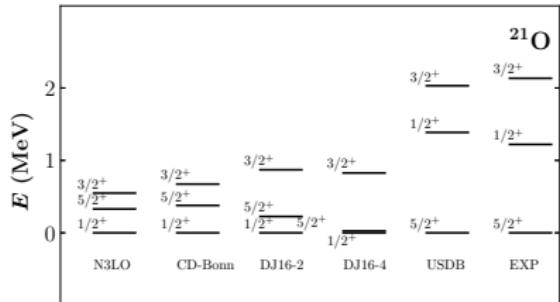
Results: *sd*-Shell Effective Interactions

► Spectra for Some *sd*-Shell Nuclei:



Results: *sd*-Shell Effective Interactions

► Spectra for Some *sd*-Shell Nuclei:



► Conclusions:

- The *sd*-shell effective interactions derived from Daejeon16 using MBPT are slightly better than N3LO and CD-Bonn in the description of nuclear binding energies and spectra.
- Effective interactions derived from MBPT have overbinding problems in the description of O isotopes.
- Enlarging the model space of MBPT can improve the overbinding problem.

► Outlook:

- Enlarging model space of MBPT
- Including 3rd order diagrams in MBPT
- Monopole correction on the effective Hamiltonian
- Including three-body interactions

Thank you